Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2021 – 11:17 am BST

PDB ID	:	7PL0
Title	:	Crystal structure of a DyP-type peroxidase 5G5 variant from Bacillus subtilis
Authors	:	Borges, P.T.; Rodrigues, C.; Silva, D.; Taborda, A.; Brissos, V.; Frazao, C.; Martins, L.O.
Deposited on	:	2021-08-27
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

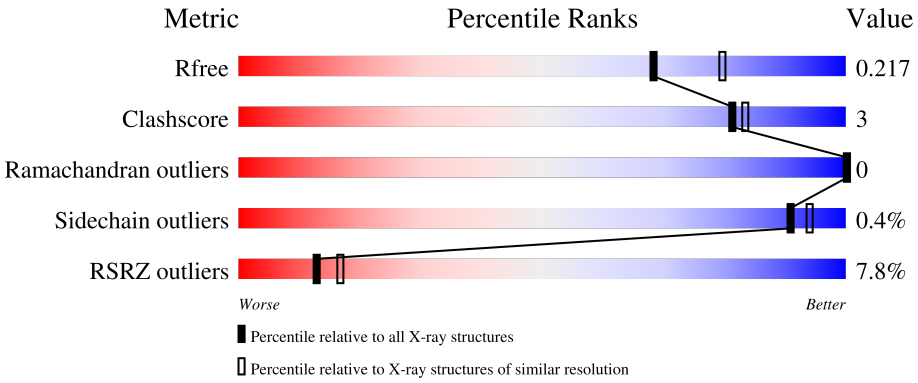
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	416	4% 78% 5% 17%
1	B	416	6% 78% · 18%
1	C	416	9% 80% · 17%
1	D	416	7% 79% 5% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11730 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

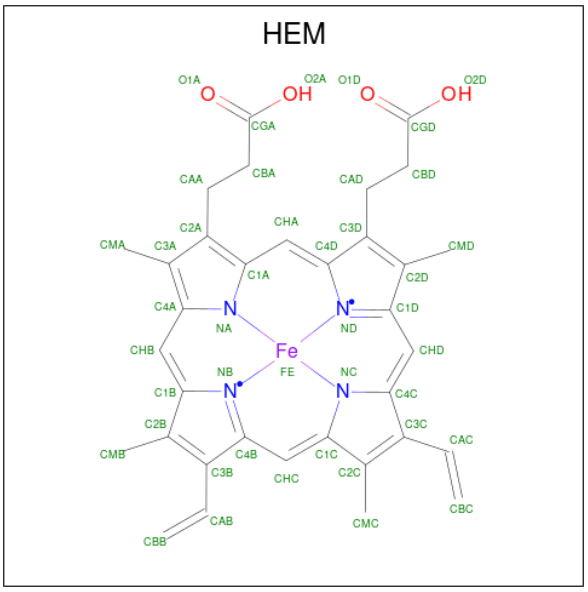
- Molecule 1 is a protein called Deferrochelatase/peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2687	1699	462	512	14			
1	B	341	Total	C	N	O	S	0	0	0
			2650	1678	456	503	13			
1	C	344	Total	C	N	O	S	0	0	0
			2673	1691	460	508	14			
1	D	349	Total	C	N	O	S	0	0	0
			2715	1718	467	517	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	GLU	LYS	engineered mutation	UNP A0A162R372
A	325	PRO	SER	engineered mutation	UNP A0A162R372
A	330	VAL	ALA	engineered mutation	UNP A0A162R372
B	317	GLU	LYS	engineered mutation	UNP A0A162R372
B	325	PRO	SER	engineered mutation	UNP A0A162R372
B	330	VAL	ALA	engineered mutation	UNP A0A162R372
C	317	GLU	LYS	engineered mutation	UNP A0A162R372
C	325	PRO	SER	engineered mutation	UNP A0A162R372
C	330	VAL	ALA	engineered mutation	UNP A0A162R372
D	317	GLU	LYS	engineered mutation	UNP A0A162R372
D	325	PRO	SER	engineered mutation	UNP A0A162R372
D	330	VAL	ALA	engineered mutation	UNP A0A162R372

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

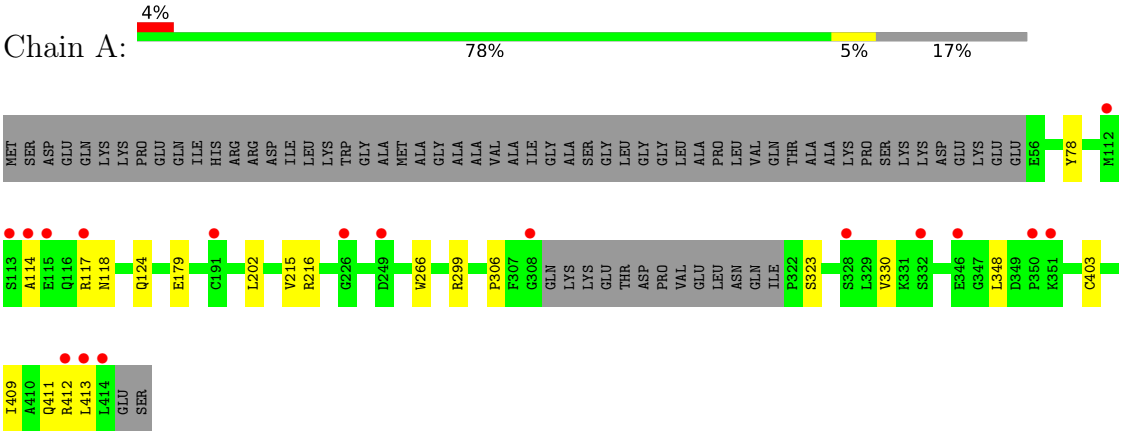
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	257	Total	O	0	0
			257	257		
3	B	220	Total	O	0	0
			220	220		
3	C	191	Total	O	0	0
			191	191		
3	D	165	Total	O	0	0
			165	165		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

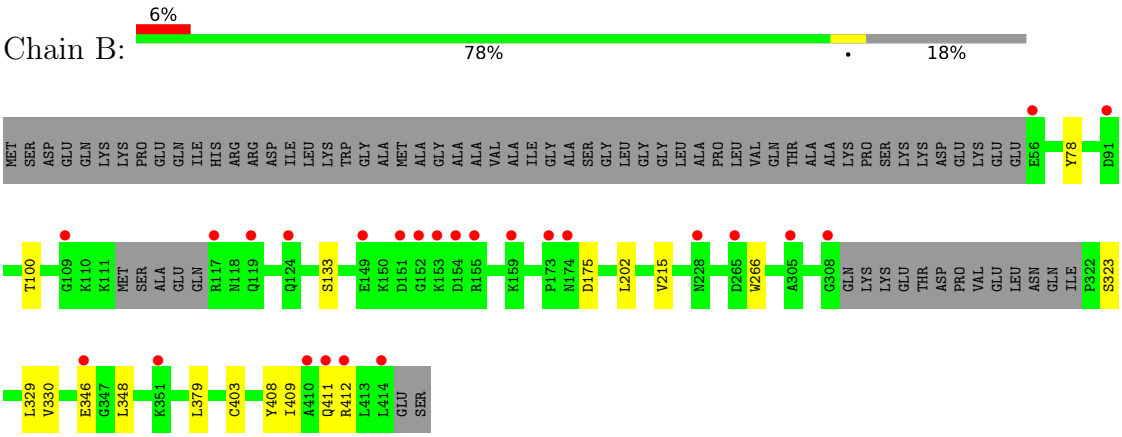
• Molecule 1: Deferrochelatase/peroxidase

Chain A:



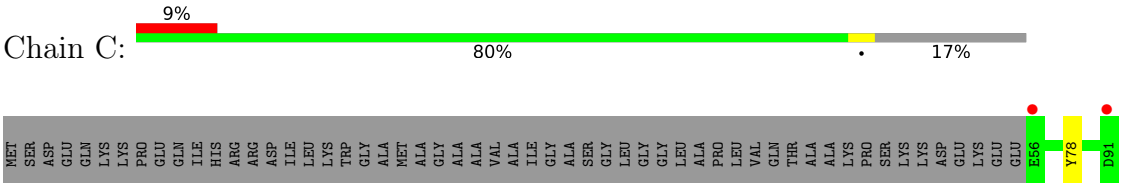
• Molecule 1: Deferrochelatase/peroxidase

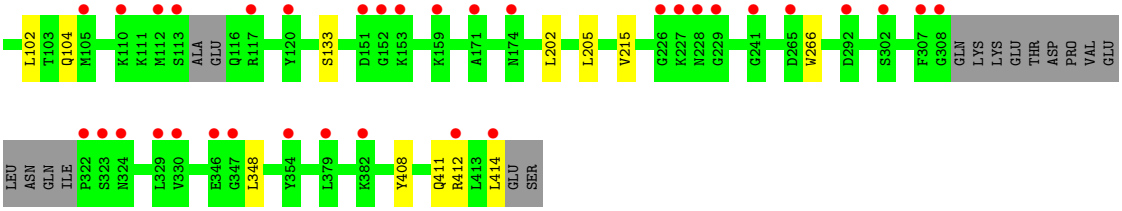
Chain B:



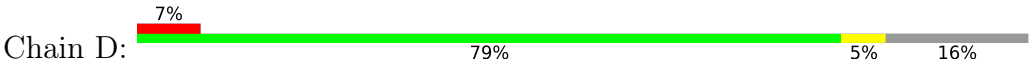
• Molecule 1: Deferrochelatase/peroxidase

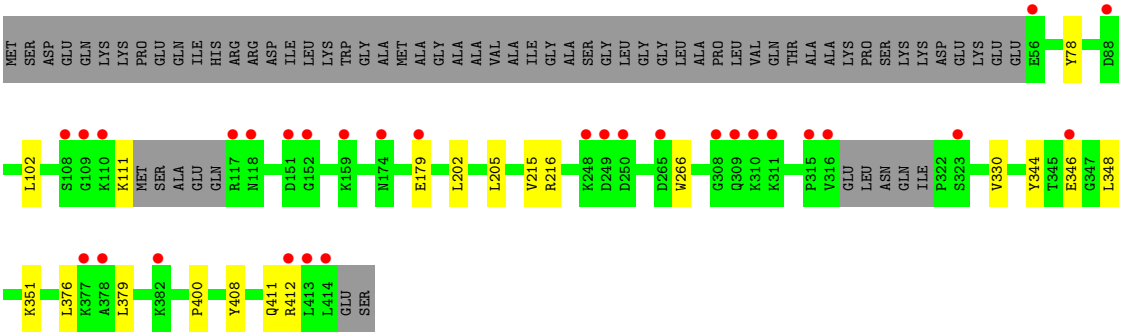
Chain C:





• Molecule 1: Deferrochelatase/peroxidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.85Å 114.76Å 116.82Å 90.00° 104.00° 90.00°	Depositor
Resolution (Å)	61.96 – 2.10 61.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (61.96-2.10) 97.1 (61.96-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.191 , 0.215 0.192 , 0.217	Depositor DCC
R_{free} test set	2005 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11730	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/2746	0.46	0/3701
1	B	0.25	0/2708	0.44	0/3649
1	C	0.26	0/2731	0.45	0/3679
1	D	0.26	0/2774	0.44	0/3738
All	All	0.26	0/10959	0.45	0/14767

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2687	0	2641	17	0
1	B	2650	0	2607	12	0
1	C	2673	0	2629	10	0
1	D	2715	0	2674	14	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	257	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	220	0	0	3	0
3	C	191	0	0	1	0
3	D	165	0	0	3	0
All	All	11730	0	10671	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:GLU:OE2	1:D:216:ARG:NH2	2.18	0.77
1:A:412:ARG:N	1:A:412:ARG:HD2	2.07	0.70
1:B:411:GLN:NE2	3:B:604:HOH:O	2.30	0.65
1:B:346:GLU:O	3:B:601:HOH:O	2.17	0.59
1:B:266:TRP:HB3	1:B:412:ARG:HB2	1.83	0.59
1:C:78:TYR:HB3	1:C:202:LEU:HD22	1.85	0.58
1:B:78:TYR:HB3	1:B:202:LEU:HD22	1.86	0.57
1:A:78:TYR:HB3	1:A:202:LEU:HD22	1.88	0.55
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.89	0.54
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.90	0.53
1:A:266:TRP:HB3	1:A:412:ARG:HB2	1.90	0.53
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.90	0.53
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.91	0.53
1:D:346:GLU:HG3	3:D:669:HOH:O	2.09	0.53
1:A:114:ALA:HB1	1:A:117:ARG:HB2	1.91	0.53
1:B:408:TYR:CE2	1:B:411:GLN:HG3	2.43	0.53
1:A:117:ARG:NH1	3:A:604:HOH:O	2.41	0.53
1:A:117:ARG:HH12	1:A:124:GLN:H	1.56	0.52
1:D:266:TRP:HB3	1:D:412:ARG:HB2	1.91	0.52
2:C:501:HEM:HMB2	2:C:501:HEM:HBB2	1.92	0.52
1:A:117:ARG:HG3	1:A:118:ASN:H	1.75	0.51
1:D:78:TYR:HB3	1:D:202:LEU:HD22	1.93	0.51
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.93	0.50
1:A:117:ARG:HG3	1:A:118:ASN:N	2.26	0.50
1:D:346:GLU:O	3:D:601:HOH:O	2.20	0.50
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.93	0.49
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.94	0.48
1:C:408:TYR:CE2	1:C:411:GLN:HG3	2.48	0.48
1:A:403:CYS:HB2	1:A:409:ILE:HD13	1.96	0.47
1:C:266:TRP:HB3	1:C:412:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:LYS:NZ	3:D:605:HOH:O	2.43	0.47
1:B:330:VAL:HG11	2:B:501:HEM:C2D	2.49	0.47
1:D:408:TYR:CE2	1:D:411:GLN:HG3	2.50	0.46
1:B:100:THR:HG21	1:B:408:TYR:HA	1.98	0.46
1:A:117:ARG:NH1	1:A:124:GLN:HG3	2.30	0.46
1:A:299:ARG:HD3	1:A:306:PRO:HA	1.98	0.46
1:A:330:VAL:HG11	2:A:501:HEM:C2D	2.52	0.45
1:A:411:GLN:C	1:A:413:LEU:H	2.19	0.45
1:A:179:GLU:OE1	1:A:216:ARG:NH2	2.46	0.45
1:D:344:TYR:HD1	1:D:346:GLU:OE1	1.99	0.45
1:C:102:LEU:HD23	1:C:205:LEU:HD23	1.99	0.45
1:C:411:GLN:O	1:C:414:LEU:HG	2.16	0.44
1:C:104:GLN:NE2	3:C:601:HOH:O	2.38	0.44
1:D:102:LEU:HD23	1:D:205:LEU:HD23	1.99	0.44
1:C:348:LEU:HD11	1:D:215:VAL:HG12	2.00	0.44
1:D:330:VAL:HG23	1:D:379:LEU:HD21	2.00	0.44
1:C:215:VAL:HG12	1:D:348:LEU:HD11	2.01	0.43
1:A:215:VAL:HG12	1:B:348:LEU:HD11	2.00	0.42
1:A:124:GLN:HE22	1:D:351:LYS:HE2	1.85	0.42
1:D:266:TRP:HE3	1:D:400:PRO:HB3	1.85	0.41
1:B:175:ASP:OD1	3:B:602:HOH:O	2.22	0.41
1:A:348:LEU:HD11	1:B:215:VAL:HG12	2.03	0.41
1:C:408:TYR:CZ	1:C:411:GLN:HG3	2.55	0.41
1:C:266:TRP:HB3	1:C:412:ARG:CG	2.51	0.41
1:B:403:CYS:HB2	1:B:409:ILE:HD13	2.03	0.41
1:B:329:LEU:HD23	1:B:379:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/416 (82%)	331 (97%)	11 (3%)	0	100	100
1	B	335/416 (80%)	325 (97%)	10 (3%)	0	100	100
1	C	338/416 (81%)	331 (98%)	7 (2%)	0	100	100
1	D	343/416 (82%)	335 (98%)	8 (2%)	0	100	100
All	All	1358/1664 (82%)	1322 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/343 (84%)	287 (100%)	1 (0%)	92	95
1	B	284/343 (83%)	282 (99%)	2 (1%)	84	88
1	C	287/343 (84%)	286 (100%)	1 (0%)	92	95
1	D	292/343 (85%)	291 (100%)	1 (0%)	92	95
All	All	1151/1372 (84%)	1146 (100%)	5 (0%)	91	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	SER
1	B	133	SER
1	B	323	SER
1	C	133	SER
1	D	376	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	B	501	1	27,50,50	1.84	5 (18%)	17,82,82	1.45	3 (17%)
2	HEM	C	501	1	27,50,50	1.85	5 (18%)	17,82,82	1.43	3 (17%)
2	HEM	A	501	1	27,50,50	1.83	5 (18%)	17,82,82	1.46	3 (17%)
2	HEM	D	501	1	27,50,50	1.82	4 (14%)	17,82,82	1.51	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1	-	0/6/54/54	-
2	HEM	C	501	1	-	0/6/54/54	-
2	HEM	A	501	1	-	0/6/54/54	-
2	HEM	D	501	1	-	0/6/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-CAC	3.85	1.55	1.47
2	A	501	HEM	C3B-CAB	3.83	1.55	1.47
2	C	501	HEM	C3B-CAB	3.82	1.55	1.47
2	A	501	HEM	C3C-CAC	3.80	1.55	1.47
2	B	501	HEM	C3C-CAC	3.79	1.55	1.47
2	D	501	HEM	C3B-CAB	3.79	1.55	1.47
2	D	501	HEM	C3C-CAC	3.78	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.76	1.35	1.40
2	B	501	HEM	C3B-CAB	3.75	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.75	1.35	1.40
2	C	501	HEM	C3B-C2B	-3.73	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.73	1.35	1.40
2	B	501	HEM	C3B-C2B	-3.70	1.35	1.40
2	A	501	HEM	C3B-C2B	-3.69	1.35	1.40
2	D	501	HEM	C3B-C2B	-3.69	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.66	1.35	1.40
2	B	501	HEM	CAA-C2A	2.09	1.55	1.52
2	C	501	HEM	CAA-C2A	2.07	1.55	1.52
2	A	501	HEM	CAA-C2A	2.02	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	CBD-CAD-C3D	-2.72	107.46	112.48
2	B	501	HEM	CBD-CAD-C3D	-2.56	107.76	112.48
2	A	501	HEM	CBD-CAD-C3D	-2.49	107.90	112.48
2	B	501	HEM	CMC-C2C-C3C	2.32	129.02	124.68
2	C	501	HEM	CMC-C2C-C3C	2.31	129.00	124.68
2	A	501	HEM	CMC-C2C-C3C	2.31	129.00	124.68
2	C	501	HEM	CMB-C2B-C3B	2.29	128.96	124.68
2	D	501	HEM	CMB-C2B-C3B	2.27	128.92	124.68
2	D	501	HEM	CMC-C2C-C3C	2.24	128.88	124.68
2	A	501	HEM	CMB-C2B-C3B	2.20	128.79	124.68
2	B	501	HEM	CMB-C2B-C3B	2.20	128.78	124.68
2	C	501	HEM	CBD-CAD-C3D	-2.15	108.51	112.48

There are no chirality outliers.

There are no torsion outliers.

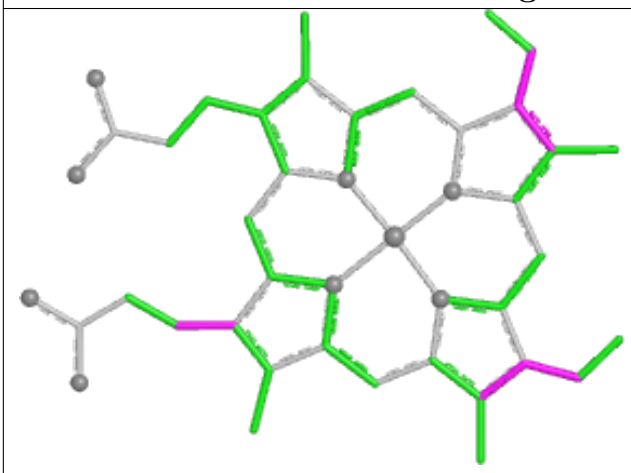
There are no ring outliers.

4 monomers are involved in 10 short contacts:

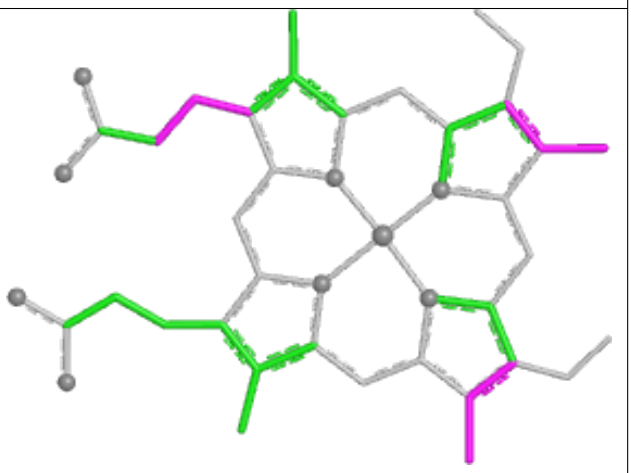
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	3	0
2	C	501	HEM	2	0
2	A	501	HEM	3	0
2	D	501	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

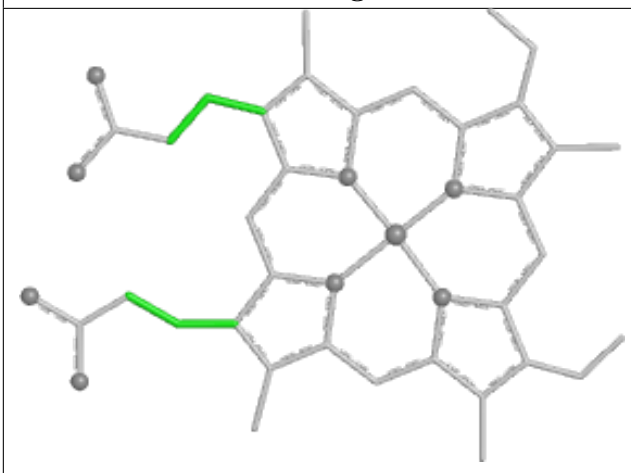
Ligand HEM B 501



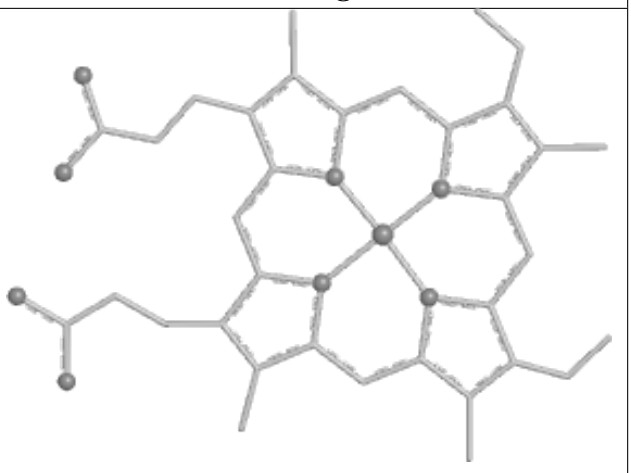
Bond lengths



Bond angles

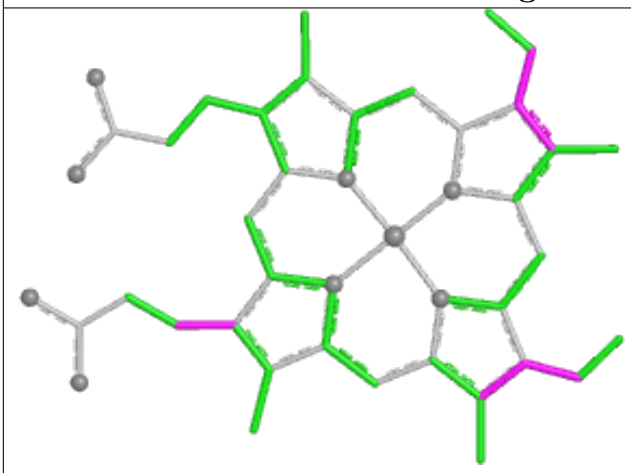


Torsions

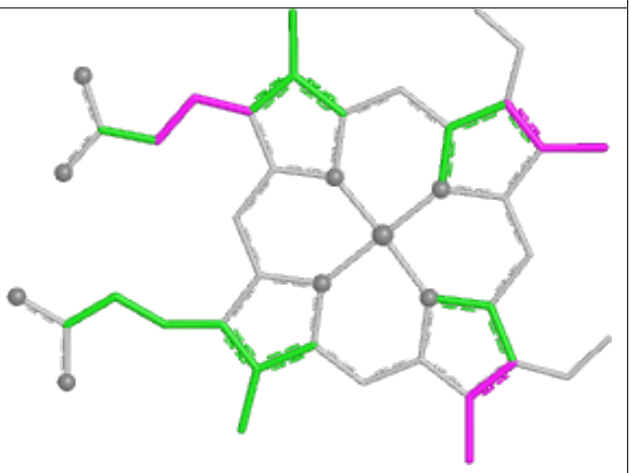


Rings

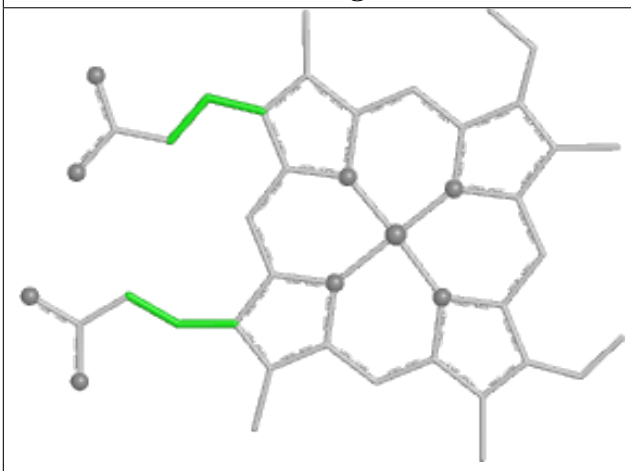
Ligand HEM C 501



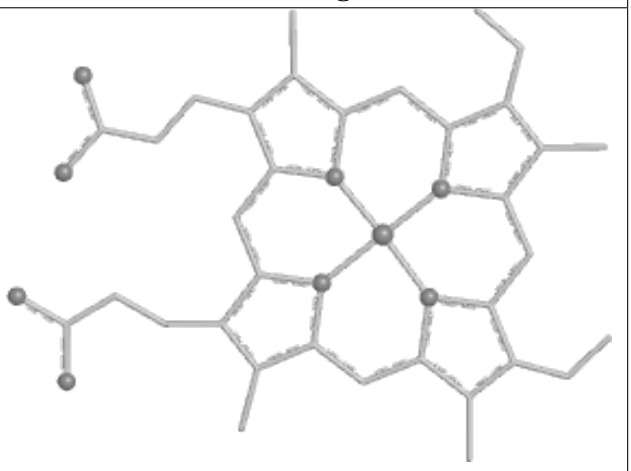
Bond lengths



Bond angles

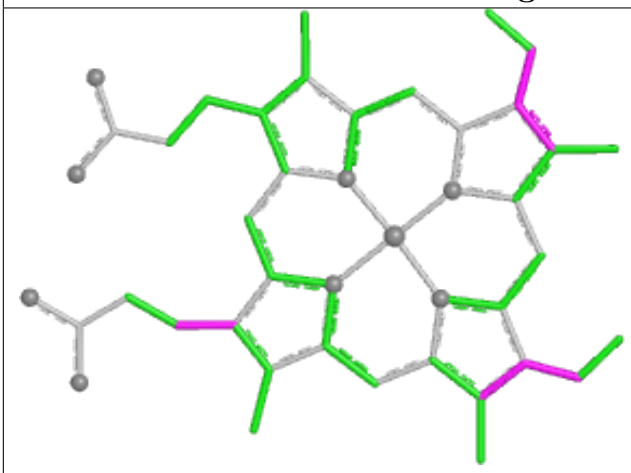


Torsions

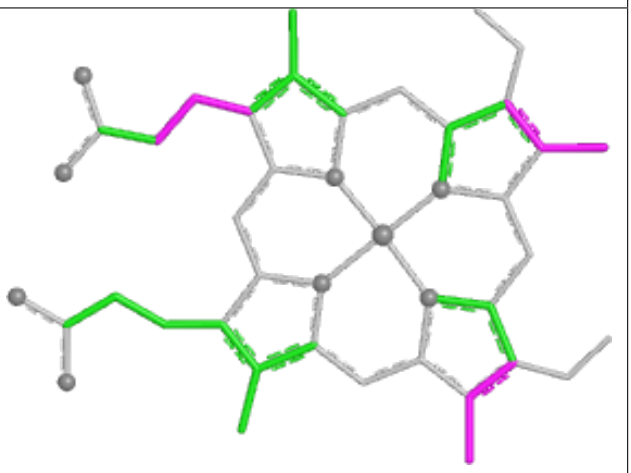


Rings

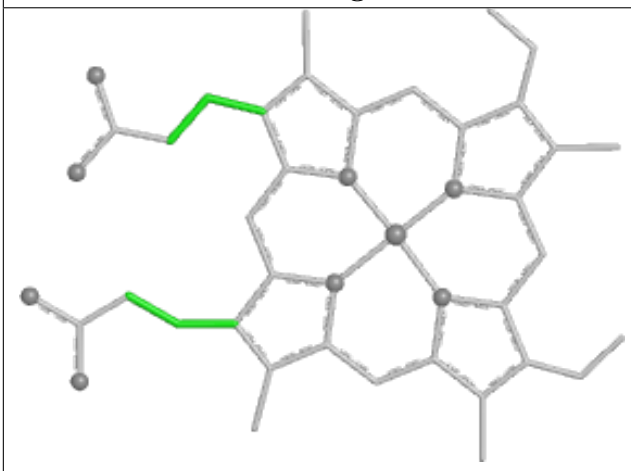
Ligand HEM A 501



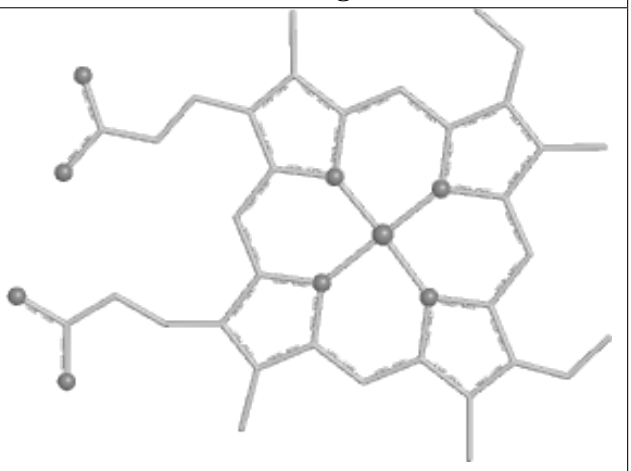
Bond lengths



Bond angles

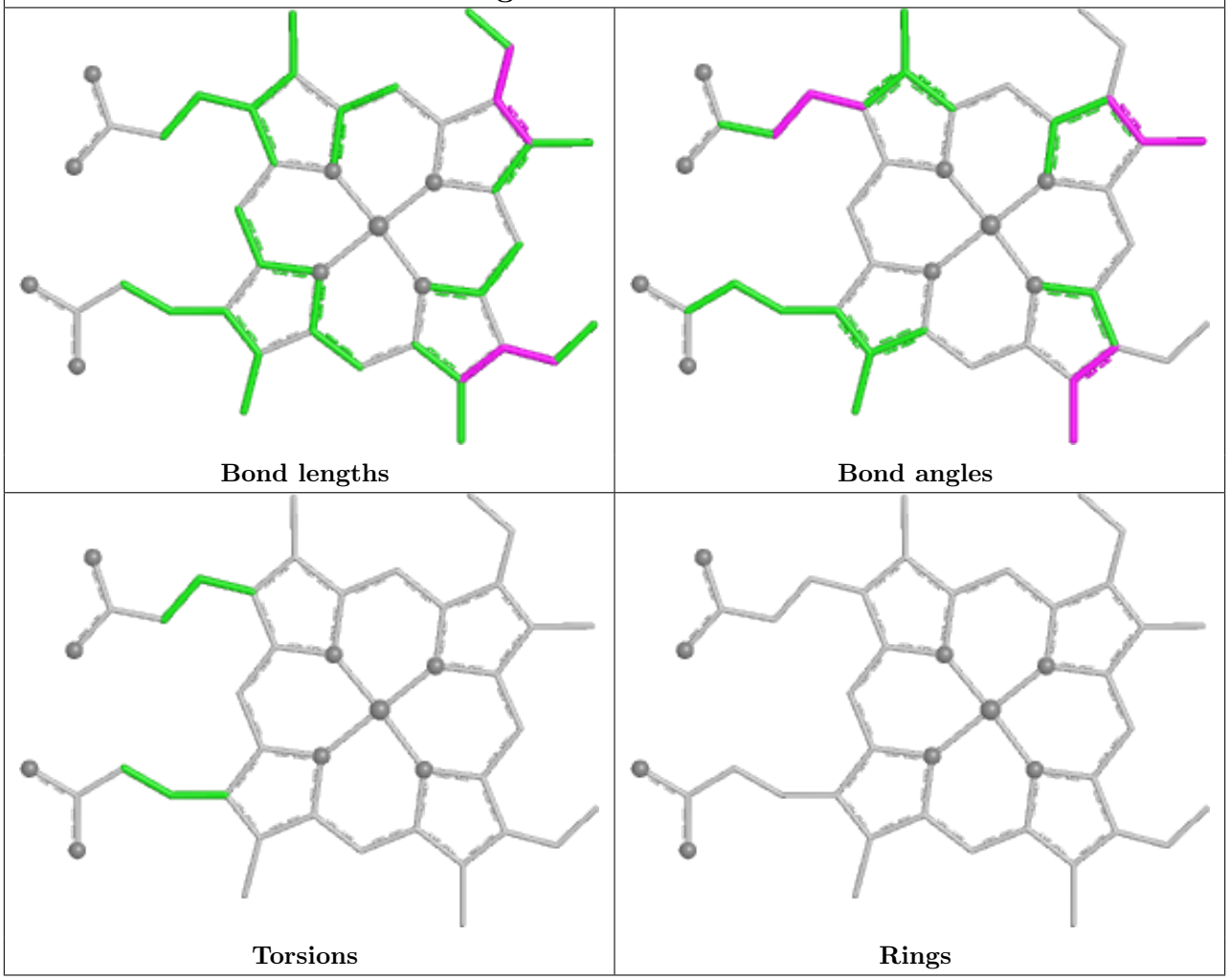


Torsions



Rings

Ligand HEM D 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	346/416 (83%)	0.72	17 (4%)	29 35	22, 34, 61, 112	0
1	B	341/416 (81%)	0.72	25 (7%)	15 19	23, 35, 65, 97	0
1	C	344/416 (82%)	0.85	36 (10%)	6 8	24, 40, 69, 98	0
1	D	349/416 (83%)	0.91	30 (8%)	10 13	26, 44, 76, 113	0
All	All	1380/1664 (82%)	0.80	108 (7%)	13 17	22, 38, 71, 113	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	308	GLY	5.8
1	B	56	GLU	5.4
1	D	118	ASN	5.3
1	A	414	LEU	4.9
1	C	307	PHE	4.8
1	C	308	GLY	4.8
1	B	308	GLY	4.7
1	D	117	ARG	4.7
1	D	346	GLU	4.5
1	D	109	GLY	4.5
1	C	113	SER	4.2
1	B	117	ARG	4.2
1	A	412	ARG	4.2
1	C	56	GLU	4.0
1	B	154	ASP	3.9
1	A	112	MET	3.9
1	A	413	LEU	3.9
1	A	226	GLY	3.9
1	B	346	GLU	3.8
1	A	114	ALA	3.8
1	A	113	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	412	ARG	3.6
1	A	115	GLU	3.5
1	C	228	ASN	3.4
1	C	414	LEU	3.3
1	D	413	LEU	3.3
1	D	152	GLY	3.2
1	D	151	ASP	3.2
1	D	159	LYS	3.2
1	C	412	ARG	3.1
1	C	302	SER	3.1
1	C	159	LYS	3.1
1	A	308	GLY	3.1
1	C	330	VAL	3.1
1	D	174	ASN	3.0
1	A	346	GLU	3.0
1	B	414	LEU	3.0
1	B	174	ASN	3.0
1	B	265	ASP	3.0
1	D	248	LYS	3.0
1	D	250	ASP	2.9
1	C	346	GLU	2.9
1	C	151	ASP	2.9
1	C	347	GLY	2.8
1	B	228	ASN	2.7
1	B	153	LYS	2.7
1	B	411	GLN	2.7
1	D	56	GLU	2.7
1	D	378	ALA	2.6
1	C	226	GLY	2.6
1	D	323	SER	2.6
1	D	108	SER	2.5
1	C	171	ALA	2.5
1	D	316	VAL	2.5
1	C	152	GLY	2.5
1	C	265	ASP	2.5
1	C	324	ASN	2.5
1	A	191	CYS	2.5
1	B	173	PRO	2.5
1	C	174	ASN	2.4
1	D	310	LYS	2.4
1	B	351	LYS	2.4
1	C	329	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	412	ARG	2.4
1	D	249	ASP	2.4
1	C	322	PRO	2.3
1	C	112	MET	2.3
1	C	153	LYS	2.3
1	D	382	LYS	2.3
1	D	315	PRO	2.3
1	B	152	GLY	2.3
1	B	305	ALA	2.3
1	C	110	LYS	2.3
1	D	311	LYS	2.3
1	A	117	ARG	2.3
1	D	377	LYS	2.3
1	A	350	PRO	2.3
1	C	323	SER	2.3
1	C	379	LEU	2.2
1	C	241	GLY	2.2
1	C	292	ASP	2.2
1	D	265	ASP	2.2
1	B	149	GLU	2.2
1	D	179	GLU	2.2
1	B	155	ARG	2.2
1	D	110	LYS	2.2
1	A	351	LYS	2.2
1	B	91	ASP	2.1
1	C	227	LYS	2.1
1	C	229	GLY	2.1
1	B	109	GLY	2.1
1	B	124	GLN	2.1
1	C	105	MET	2.1
1	C	382	LYS	2.1
1	B	151	ASP	2.1
1	A	328	SER	2.1
1	A	249	ASP	2.1
1	B	159	LYS	2.1
1	C	117	ARG	2.0
1	B	410	ALA	2.0
1	C	91	ASP	2.0
1	D	414	LEU	2.0
1	A	332	SER	2.0
1	D	309	GLN	2.0
1	C	120	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	354	TYR	2.0
1	B	119	GLN	2.0
1	D	88	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

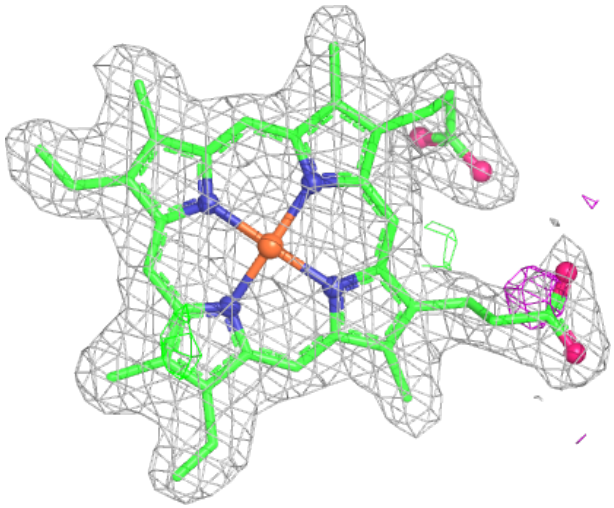
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

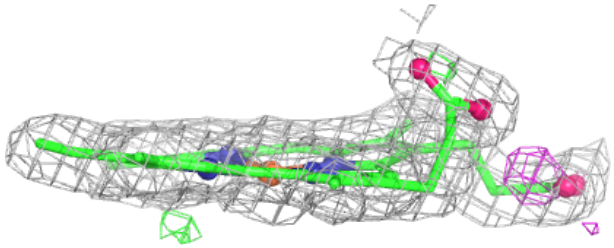
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	C	501	43/43	0.89	0.16	30,32,38,39	0
2	HEM	D	501	43/43	0.90	0.15	32,36,44,47	0
2	HEM	B	501	43/43	0.92	0.15	22,25,29,31	0
2	HEM	A	501	43/43	0.94	0.15	22,25,28,29	0

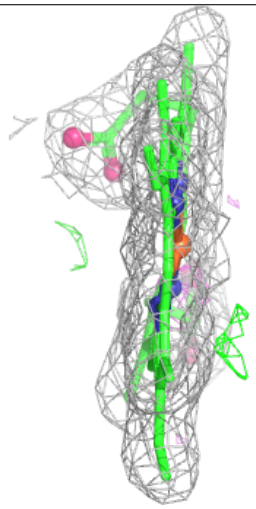
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

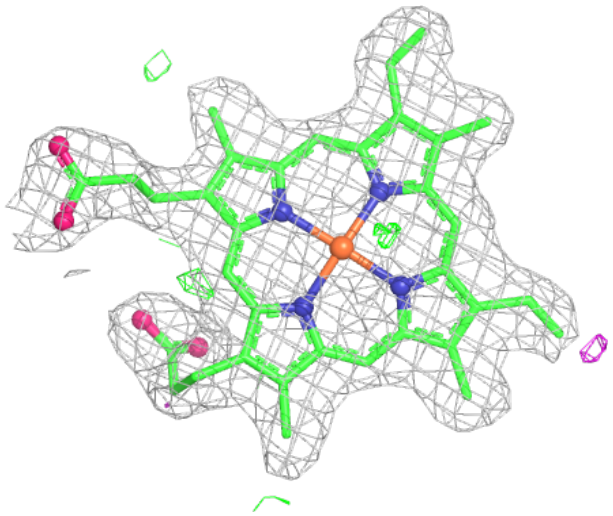


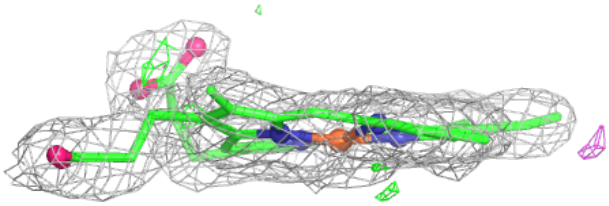


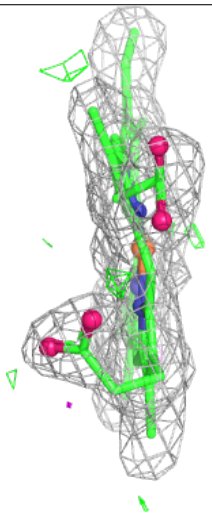


Electron density around HEM D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

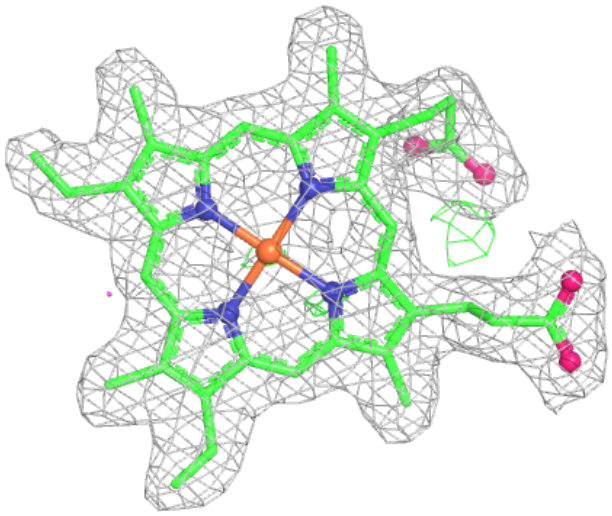


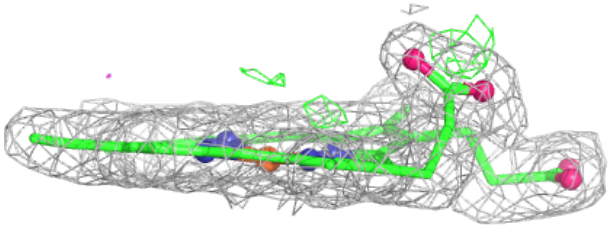


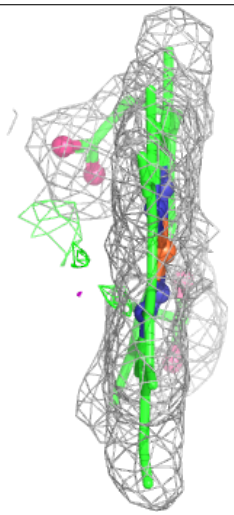


Electron density around HEM B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

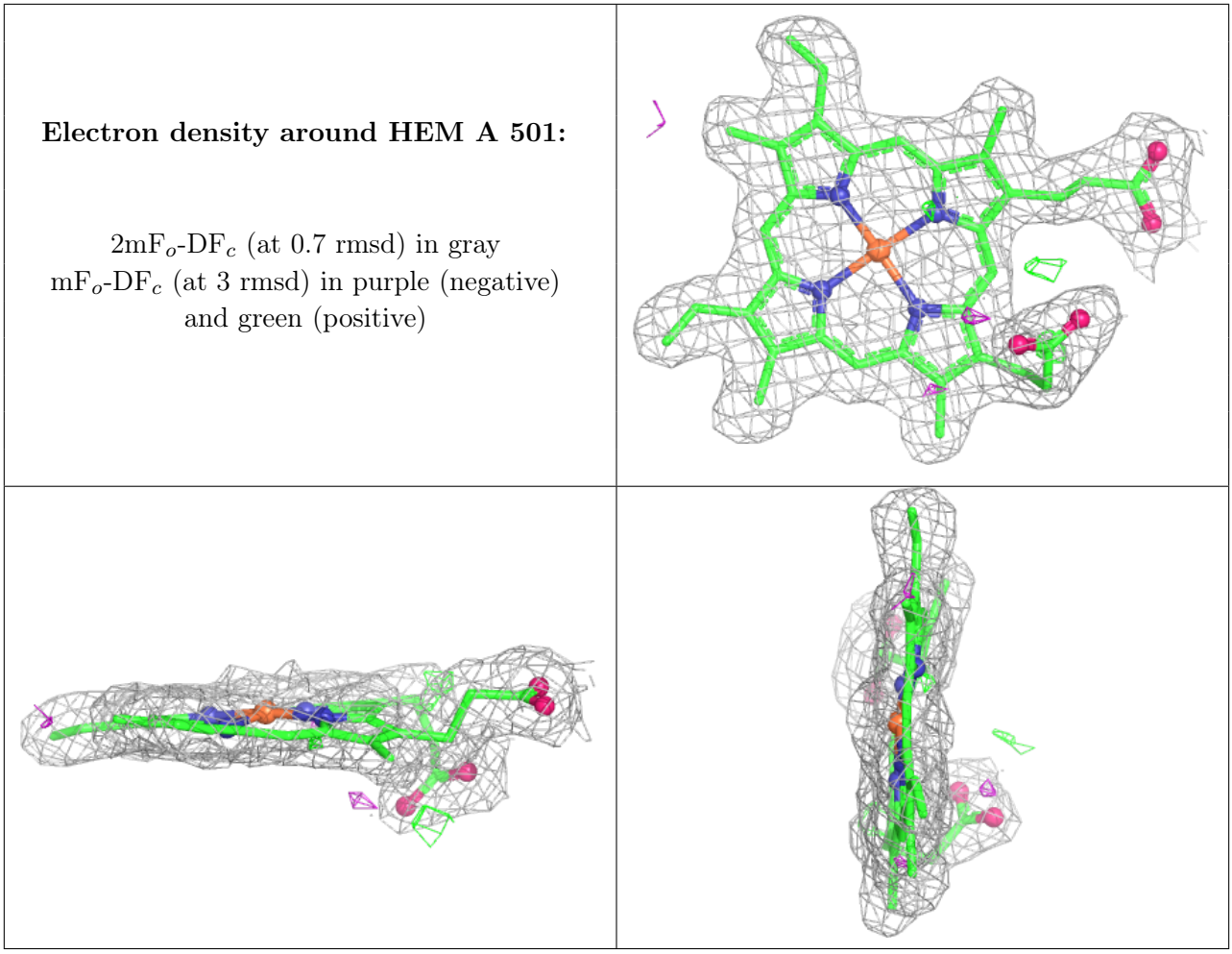






Electron density around HEM A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.